Jiang Hualiang

List of Publications by Year
in descending order

82 papers	8,849 citations	159585 30 h-index	60623 81 g-index
89 all docs	89 docs citations	89 times ranked	13190 citing authors

#	Article	IF	Citations
1	Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature, 2020, 582, 289-293.	27.8	3,133
2	Structure-based design of antiviral drug candidates targeting the SARS-CoV-2 main protease. Science, 2020, 368, 1331-1335.	12.6	1,135
3	Structural basis for inhibition of the RNA-dependent RNA polymerase from SARS-CoV-2 by remdesivir. Science, 2020, 368, 1499-1504.	12.6	950
4	Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614.	12.6	454
5	Structures of the Omicron spike trimer with ACE2 and an anti-Omicron antibody. Science, 2022, 375, 1048-1053.	12.6	216
6	Cinanserin Is an Inhibitor of the 3C-Like Proteinase of Severe Acute Respiratory Syndrome Coronavirus and Strongly Reduces Virus Replication In Vitro. Journal of Virology, 2005, 79, 7095-7103.	3.4	185
7	SHAFTS: A Hybrid Approach for 3D Molecular Similarity Calculation. 1. Method and Assessment of Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 2372-2385.	5.4	145
8	Artificial intelligence in drug design. Science China Life Sciences, 2018, 61, 1191-1204.	4.9	145
9	Structural insights into the human D1 and D2 dopamine receptor signaling complexes. Cell, 2021, 184, 931-942.e18.	28.9	140
10	Structural insights into the lipid and ligand regulation of serotonin receptors. Nature, 2021, 592, 469-473.	27.8	138
11	Identification of pyrogallol as a warhead in design of covalent inhibitors for the SARS-CoV-2 3CL protease. Nature Communications, 2021, 12, 3623.	12.8	111
12	Structure of the glucagon receptor in complex with a glucagon analogue. Nature, 2018, 553, 106-110.	27.8	109
13	Structural basis for inhibition of the SARS-CoV-2 RNA polymerase by suramin. Nature Structural and Molecular Biology, 2021, 28, 319-325.	8.2	104
14	SARS-CoV-2 envelope protein causes acute respiratory distress syndrome (ARDS)-like pathological damages and constitutes an antiviral target. Cell Research, 2021, 31, 847-860.	12.0	102
15	Facile Creation of 3â€Indolylâ€3â€hydroxyâ€2â€oxindoles by an Organocatalytic Enantioselective Friedelâ€“Crafts Reaction of Indoles with Isatins. Advanced Synthesis and Catalysis, 2010, 352, 833-838.	4.3	92
16	A Direct Amineâ€Palladium Acetate Cocatalyzed Saegusa Oxidation Reaction of Unmodified Aldehydes to Î±,Î²â€Unsaturated Aldehydes. Advanced Synthesis and Catalysis, 2009, 351, 1229-1232.	4.3	88
17	Free energy landscape for the binding process of Huperzine A to acetylcholinesterase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4273-4278.	7.1	79
18	Small-Molecule Targeting of E3 Ligase Adaptor SPOP in Kidney Cancer. Cancer Cell, 2016, 30, 474-484.	16.8	74

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19	Graph neural networks for automated de novo drug design. Drug Discovery Today, 2021, 26, 1382-1393.	6.4	71
20	Design and development of an oral remdesivir derivative VV116 against SARS-CoV-2. Cell Research, 2021, 31, 1212-1214.	12.0	71
21	High-resolution mapping of brain vasculature and its impairment in the hippocampus of Alzheimer's disease mice. National Science Review, 2019, 6, 1223-1238.	9.5	65
22	Silverâ€Catalyzed Intramolecular Cyclization of oâ€(1â€Alkynyl)benzamides: Efficient Synthesis of (1H)â€Isochromenâ€1â€imines. Advanced Synthesis and Catalysis, 2009, 351, 2605-2610.	4.3	57
23	Structural basis for activation of the growth hormone-releasing hormone receptor. Nature Communications, 2020, 11, 5205.	12.8	57
24	Goldâ€•and Silverâ€Catalyzed Intramolecular Hydroamination of Terminal Alkynes: Waterâ€Triggered Chemoâ€• and Regioselective Synthesis of Fused Tricyclic Xanthines. Advanced Synthesis and Catalysis, 2009, 351, 2770-2778.	4.3	55
25	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. Bioinformatics, 2015, 31, 2049-2051.	4.1	52
26	Design, Synthesis, and Biological Evaluation of Peptidomimetic Aldehydes as Broad-Spectrum Inhibitors against Enterovirus and SARS-CoV-2. Journal of Medicinal Chemistry, 2022, 65, 2794-2808.	6.4	52
27	Structures of full-length glycoprotein hormone receptor signalling complexes. Nature, 2021, 598, 688-692.	27.8	52
28	Structures of the human dopamine D3 receptor-Gi complexes. Molecular Cell, 2021, 81, 1147-1159.e4.	9.7	51
29	Mechanism of dopamine binding and allosteric modulation of the human D1 dopamine receptor. Cell Research, 2021, 31, 593-596.	12.0	48
30	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	10.5	38
31	Computational Studies on Acetylcholinesterases. Molecules, 2017, 22, 1324.	3.8	33
32	Effects of Shuanghuanglian oral liquids on patients with COVID-19: a randomized, open-label, parallel-controlled, multicenter clinical trial. Frontiers of Medicine, 2021, 15, 704-717.	3.4	33
33	Estimation of acute oral toxicity in rat using local lazy learning. Journal of Cheminformatics, 2014, 6, 26.	6.1	30
34	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	6.1	30
35	Protein tyrosine phosphatase receptor U (PTPRU) is required for glioma growth and motility. Carcinogenesis, 2014, 35, 1901-1910.	2.8	30
36	Combinatorial Pharmacophore-Based 3D-QSAR Analysis and Virtual Screening of FGFR1 Inhibitors. International Journal of Molecular Sciences, 2015, 16, 13407-13426.	4.1	26

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37	Pharmacokinetics-Driven Optimization of 4(3H)-Pyrimidinones as Phosphodiesterase Type 5 Inhibitors Leading to TPN171, a Clinical Candidate for the Treatment of Pulmonary Arterial Hypertension. Journal of Medicinal Chemistry, 2019, 62, 4979-4990.	6.4	25
38	Automated design and optimization of multitarget schizophrenia drug candidates by deep learning. European Journal of Medicinal Chemistry, 2020, 204, 112572.	5.5	25
39	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
40	A Genetic Algorithm Based Support Vector Machine Model for Blood-Brain Barrier Penetration Prediction. BioMed Research International, 2015, 2015, 1-13.	1.9	23
41	Molecular basis for allosteric agonism and G protein subtype selectivity of galanin receptors. Nature Communications, 2022, 13, 1364.	12.8	23
42	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. Journal of Chemical Theory and Computation, 2009, 5, 1411-1420.	5.3	22
43	Ionicâ€Liquidâ€Supported Total Synthesis of Sansalvamide A Peptide. Synthetic Communications, 2008, 38, 239-248.	2.1	20
44	Nature brings new avenues to the therapy of central nervous system diseasesâ€”An overview of possible treatments derived from natural products. Science China Life Sciences, 2019, 62, 1332-1367.	4.9	20
45	Structural basis of leukotriene B4 receptor 1 activation. Nature Communications, 2022, 13, 1156.	12.8	19
46	Transformation of Aryl Acyloin Oâ€Alkyl and Oâ€Phenyl Derivatives to Ketones. Synthetic Communications, 2007, 37, 149-156.	2.1	18
47	Probing the structure and dynamics of caveolin-1 in a caveolae-mimicking asymmetric lipid bilayer model. European Biophysics Journal, 2016, 45, 511-521.	2.2	18
48	The Mechanism by Which Luteolin Disrupts the Cytoplasmic Membrane of Methicillin-Resistant Staphylococcus aureus. Journal of Physical Chemistry B, 2018, 122, 1427-1438.	2.6	18
49	Potential treatment of COVID-19 by inhibitors of human dihydroorotateÂdehydrogenase. Protein and Cell, 2020, 11, 699-702.	11.0	18
50	Drug target inference by mining transcriptional data using a novel graph convolutional network framework. Protein and Cell, 2022, 13, 281-301.	11.0	18
51	Facing small and biased data dilemma in drug discovery with enhanced federated learning approaches. Science China Life Sciences, 2022, 65, 529-539.	4.9	17
52	Design, Synthesis, and Biological Evaluation of Novel Nonsteroidal Farnesoidâ€…X Receptor (FXR) Antagonists: Molecular Basis of FXR Antagonism. ChemMedChem, 2015, 10, 1184-1199.	3.2	16
53	Discovery of Novel Small Molecule Anti-HCV Agents via the CypA Inhibitory Mechanism Using O-Acylation-Directed Lead Optimization. Molecules, 2015, 20, 10342-10359.	3.8	16
54	Structure-Based Design of Dual-Acting Compounds Targeting Adenosine A_{2A} Receptor and Histone Deacetylase as Novel Tumor Immunotherapeutic Agents. Journal of Medicinal Chemistry, 2021, 64, 16573-16597.	6.4	16

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55	Allostery in Drug Development. Advances in Experimental Medicine and Biology, 2019, 1163, 1-23.	1.6	15
56	Dynamic modifications of biomacromolecules: mechanism and chemical interventions. Science China Life Sciences, 2019, 62, 1459-1471.	4.9	14
57	Oral remdesivir derivative VV116 is a potent inhibitor of respiratory syncytial virus with efficacy in mouse model. Signal Transduction and Targeted Therapy, 2022, 7, 123.	17.1	14
58	China's reform of the regulatory system for medical products and its impact. National Science Review, 2019, 6, 1-1.	9.5	13
59	Constitutive signal bias mediated by the human GHRHR splice variant 1. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	13
60	Microwaveâ€Assisted Dehalogenation of Î±â€Haloketones by Zinc and Ammonium Chloride in Alcohol. Synthetic Communications, 2008, 38, 567-575.	2.1	12
61	Discovery of new antimalarial agents: Second-generation dual inhibitors against FP-2 and PfDHFR via fragments assembely. Bioorganic and Medicinal Chemistry, 2017, 25, 6467-6478.	3.0	12
62	Beneficial effects exerted by hydroxychloroquine in treating COVID-19 patients via protecting multiple organs. Science China Life Sciences, 2021, 64, 330-333.	4.9	12
63	Why is the SARS-CoV-2 Omicron variant milder?. Innovation(China), 2022, 3, 100251.	9.1	12
64	Identification, synthesis and pharmacological evaluation of novel anti-EV71 agents via cyclophilin A inhibition. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5682-5686.	2.2	11
65	Cation sitting in aromatic cages:ab initio computational studies on tetramethylammoniumâ€“(benzene)n (n=3â€“4) complexes. Journal of Physical Organic Chemistry, 2007, 20, 448-453.	1.9	10
66	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. Journal of Medicinal Chemistry, 2020, 63, 6523-6537.	6.4	10
67	Drug discovery and development targeting the life cycle of SARS-CoV-2. Fundamental Research, 2021, 1, 151-165.	3.3	9
68	Techniques used for the discovery of therapeutic compounds: The case of SARS. Drug Discovery Today: Technologies, 2006, 3, 277-283.	4.0	8
69	Effects of ion interactions with a cholesterol-rich bilayer. Biochemical and Biophysical Research Communications, 2015, 468, 125-129.	2.1	8
70	Discovery of potent 2,4-difluoro-linker poly(ADP-ribose) polymerase 1 inhibitors with enhanced water solubility and in vivo anticancer efficacy. Acta Pharmacologica Sinica, 2017, 38, 1521-1532.	6.1	8
71	The open-close mechanism of M2 channel protein in influenza A virus: A computational study on the hydrogen bonds and cation-Ï€ interactions among His37 and Trp41. Science in China Series B: Chemistry, 2008, 51, 768-775.	0.8	6
72	Computational characterization of transducer recognition of Î²2 adrenergic receptor. Biochemical and Biophysical Research Communications, 2022, 592, 67-73.	2.1	6

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73	Accelerating All-Atom Normal Mode Analysis with Graphics Processing Unit. Journal of Chemical Theory and Computation, 2011, 7, 1595-1603.	5.3	5
74	Characterizing the interactions of two lipid modifications with lipid rafts: farnesyl anchors vs. palmitoyl anchors. European Biophysics Journal, 2018, 47, 19-30.	2.2	5
75	Dual-acting antitumor agents targeting the A2A adenosine receptor and histone deacetylases: Design and synthesis of 4-(furan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine derivatives. European Journal of Medicinal Chemistry, 2022, 236, 114326.	5.5	5
76	Refinement and 3Dâ€QSAR Studies of Inhibitors of Cyclophilin A Containing Amide Linker. QSAR and Combinatorial Science, 2009, 28, 183-193.	1.4	4
77	Discovery of Benzylidene Derivatives as Potent Syk Inhibitors: Synthesis, SAR Analysis, and Biological Evaluation. Archiv Der Pharmazie, 2015, 348, 463-474.	4.1	4
78	Structural insights into ligand binding and activation of the human thyrotropin-releasing hormone receptor. Cell Research, 2022, 32, 855-857.	12.0	4
79	First Reaction of a Chiral Glyâ€Ni(II) Complex in Water. Chinese Journal of Chemistry, 2010, 28, 422-428.	4.9	3
80	Targeting sorting nexin 10 improves mouse colitis via inhibiting PIKfyve-mediated TBK1/c-Rel signaling activation. Pharmacological Research, 2021, 169, 105679.	7.1	3
81	Cryo-EM structure determination captures new chemical modification of protein. Science China Life Sciences, 2021, 64, 1781-1783.	4.9	1
82	Focused Library Design Based on Hit and Target Structures: Method and Application in Drug Discovery. , 0, , 108-124.		0